Effective interactions and operators from coupled-cluster theory

Gustav R. Jansen
Gustav.Jansen@utk.edu

ICNT: Theory for open-shell nuclei near the limits of stability
Outline

• Motivation
• Coupled-cluster theory
• Coupled-cluster effective interaction (CCEI)
• Results
• Work in progress
• Outlook
Overview

- Arrive at a Hamiltonian (a “standard model”) of nuclear physics
- Understand the link between (Lattice) QCD and EFT and nuclei
- What are the limits for the existence of nuclei (i.e. drip line location)
- Explain collective phenomena from individual motion of nuclei
- Error estimates of computed quantities
- …
The nuclear Schrödinger equation

\[ H\Psi = E\Psi \]

1. We don’t know the Hamiltonian!
2. We can’t solve the equation!
Chiral effective field theory (χEFT)

LO

NLO

NNLO

N3LO

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Computing the interaction

- Not possible to do “on the fly”.
- Three-nucleon forces takes weeks to transform to single particle coordinates.

The interaction elements have to be stored in memory!
Memory usage

Graph showing memory usage for different configurations and energy shells.

- Full storage
- Nonzero
- Titan memory
- Threebody full
- Spherical nonzero
- Spherical threebody
Three nucleons forces

- Hartree-Fock with full three-nucleon force
  - Current limit: Nmax=14, E3max=18
    - ~10 TB total memory
    - Titan : 10-20% for 1 hour
    - Need larger modelspaces beyond $^{52}Ca$

- Normal-ordered twobody approximation (NO2B)
  - Keep only contributions to:
    - Vacuum energy
    - Onebody operator
    - Twobody operator

- Residual three-nucleon force with $T_3^{(1)}$ (MBPT2).
  - 1 % effect (0.1 MeV per Nucleon)
The nuclear Schrödinger equation

\[ H\Psi = E\Psi \]

1. We don’t know the Hamiltonian!
2. We can’t solve the equation!
The basis

Quantum mechanics → Fermions

\[
\begin{pmatrix} N \\ A \end{pmatrix}
\]
Basis size

- He4
- C12
- O16
- Ca40
- Titan 1s
- Titan 1h
- Titan 1y
- Titan U

Number of states
Strategy (NUCCOR)

• Large set of single-particle states
  – Extrapolate to infinity (if possible)
• Two- and three-nucleon interaction
• Treat all nucleons identically
• Find invariant subspaces
  – Isospin projection
  – Total parity
  – Total angular momentum
• Restrict basis set (2p2h, 3p3h, …)
• Reduce the number of nucleons (CCEI)
  – Frozen core
  – Effective interactions
  – Effective operators
NUCCOR organization

- Accepted CAAR project for CORAL
  - Will run at OLCF, ALCF and NERSC
- Runs on Titan
  - INCITE project for Nuclear Structure and Reactions
- Written in Fortran
  - MPI + OpenMP
  - 100,000 lines of code
    - F77/F95/F2003/F2008
    - Pre- and post-processing in Python
  - Stand-alone IO library (Fortran, C, & Python)
- Challenges
  - Calculating the three-nucleon interaction
  - Hartree Fock/CC with three-nucleon forces
  - Equation of motion (eigenvalue problem using Arnoldi/Non-symmetric Lanczos)

Public version available 2015/2016
Closed (sub-)shell nuclei

**Coupled-cluster summary**

\[ |\Psi\rangle = e^T |\Phi_0\rangle \]

\[ T = T_h^p + T_{2h}^{2p} + T_{3h}^{3p} + \cdots \]

\[ \overline{H} = e^{-T} H e^T \]

---

**CCSD**

\[
\begin{array}{cccc}
0 & 1p1h & 2p2h & 3p3h \\
E_{CC} & 0 & 0 & 0 \\
1p1h & 0 & 0 & 0 \\
2p2h & 0 & 0 & 0 \\
3p3h & 0 & 0 & 0 \\
\end{array}
\]

**CCSDT**

\[
\begin{array}{cccc}
0 & 1p1h & 2p2h & 3p3h \\
E_{CC} & 0 & 0 & 0 \\
1p1h & 0 & 0 & 0 \\
2p2h & 0 & 0 & 0 \\
3p3h & 0 & 0 & 0 \\
\end{array}
\]
Example: $^{48}\text{Ti}$

![Graph showing harmonic oscillator amplitudes for $^{48}\text{Ti}$ with current limit.]
NUCCOR coverage (PA/PR)
One particle attached or removed

\[ \overline{H} = e^{-T H e^T} \]

\[ R^{A+1} = R^p + R^{2p}_h + R^{3p}_{2h} + R^{4p}_{3h} + \cdots \]

\[ R^{A-1} = R_h + R^{p}_{2h} + R^{2p}_{3h} + R^{3p}_{4h} + \cdots \]
NUCCOR coverage (2PA/2PR)
Two particles attached or removed

\[ \overline{H} = e^{-T}He^T \]

\[ R^{A+2} = R^{2p} + R^{3p} + R^{4p} + R^{5p} + \ldots \]

\[ R^{A-2} = R^{2h} + R^{3h} + R^{4h} + R^{5h} + \ldots \]
Example: 2PA
Coupled-cluster effective interaction (CCEI)

Decide on a valence space $V$.

Need a twobody interaction in $V$ that reproduce a set of chosen eigenvalues.

Find as many eigenpairs $(R_{\mu}^{A+2}, E_{\mu})$ in the full space, as there are twobody configurations in $V$.

Project the full eigenvectors onto $V$ to find the eigenvectors of the effective Hamiltonian $\mathcal{H}$.

Construct $\mathcal{H}$ using its eigenpairs.

Final symmetric Hamiltonian after a symmetric orthogonalization step.

\[ \overline{H} R_{\mu}^{A+2} = E_{\mu} R_{\mu}^{A+2} \]

\[ V = \begin{bmatrix} R'_{1} & R'_{2} & \cdots & R'_{n} \end{bmatrix} \]

\[ \mathcal{H} = V^{-1} EV \]

\[ \Theta = V^{-1} \overline{O} V \]
**Bloch-Brandow effective interaction (Lee-Suzuki similarity transformation)**

Solve for the $A_c+2$ problems via two-particle attached equation-of-motion coupled-cluster

$$
\bar{H} R_{\mu}^{A_c+2} \Phi_0 = \omega_\mu R_{\mu}^{A_c+2} \Phi_0
$$

$$
\langle \Phi_0 | L_{\mu}^{A_c+2} \bar{H} \rangle = \omega_\mu \langle \Phi_0 | L_{\mu}^{A_c+2} \rangle
$$

To obtain $H_{\text{eff}}$ we can either project the left or the right solutions onto the $P$-space:

$$
| \psi_{k}^{\text{eff}} \rangle \equiv P | R^{A,A_c+2} \rangle
$$

Using the right eigenvector projections we obtain CCEI:

$$
\langle \alpha_P | \bar{H}_{\text{eff}}^{A,A_c+2} | \alpha_{P'} \rangle = \sum_{k=1}^{d} \langle \alpha_P | R_k^{A,A_c+2} \rangle e_k \langle \alpha_{P'} | R_k^{A,A_c+2} \rangle
$$

We can hermitize $H_{\text{CCEI}}$ by using the operator $S$ that diagonalizes $H_{\text{CCEI}}$

$$
\left[ S^\dagger S \right]^{1/2} \bar{H}_{\text{CCEI}}^{A} \left[ S^\dagger S \right]^{-1/2}
$$
CCEI: Application to the oxygen chain


- Start from chiral NN(N3LO$_{EM}$) + 3NF(N2LO) interactions SRG evolved to 2.0fm$^{-1}$
- Model space size $N_{\text{max}} = E_{3\text{max}} = 12$, $h\omega = 20\text{MeV}$

Low-lying states in $^{17}$O as a function of $A$. These energies defines the single-particle energies of $H_{\text{eff}}$

- Diagonalize the effective hamiltonian in the valence space.

\[
\begin{align*}
\text{Q} & \quad \text{P} \\
\text{Q} & \quad \text{Q} \\
\text{P} & \quad \text{P} \\
\text{Q} & \quad \text{Q} \\
\text{Q} & \quad \text{Q} \\
\vdots & \quad \text{P} \\
p_{3/2} & \quad f_{7/2} \\
d_{3/2} & \quad s_{1/2} \\
d_{5/2} & \quad p_{1/2} \\
p_{3/2} & \quad s_{1/2}
\end{align*}
\]
CCEI: Application to the oxygen chain


Comparison between coupled-cluster effective interaction (CCEI) and “exact” coupled-cluster.
Coupled-cluster effective interactions for the shell model: Oxygen isotopes
Coupled-cluster effective interactions for the shell model: Carbon isotopes
Binding energies

![Graph showing binding energies for different elements.](image-url)
Extending CCEI to open-shell and deformed nuclei: $^{20,24}\text{Ne}$ and $^{23,24}\text{Mg}$
Extending CCEI to open-shell and deformed nuclei: $^{20,24}$Ne and $^{23,24}$Mg
CCEI: Source of uncertainty

- Single particle energies
  - How are these calculated?
  - Need more correlations in the wavefunctions?
  - Continuum degrees of freedom.

- A+2 body wavefunctions
  - Freedom in which eigenvectors to choose.
    - Lowest energy or largest overlap with valence space.
  - Different level of convergence.
  - Center-of-mass effects.

- Valence space
  - Larger valence space?
  - Uncontrolled projection.
Effective operator: Point proton radius

![Graph showing effective interactions and operators from coupled-cluster theory]

- **Effective operator**: Point proton radius

- **Graph legend**:
  - Onebody only
  - Onebody and twobody
  - CC

- **X-axis**: Mass
- **Y-axis**: $R^2$
## Challenges

- Three-nucleon forces in HF, CC and EOM-CC.
  - Residual three-nucleon forces contribute > 1%
  - Needs to be included in CC.
- Additional correlations in EOM-CC.
  - Not possible to include the full set of amplitudes.
  - Active spaces?
- Larger modelspaces (three-nucleon force).
  - $N_{\text{max}}=14$, $E_{3\text{max}}=18$ not enough
  - Quickly saturates the available computational resources.
- Cross shell effective interactions and operators
  - Computation of A+2-body wavefunctions is the bottleneck.
Outlook

• Bigger, better, faster
  – More memory (three-nucleon forces)
  – Better algorithms and use of accelerators
  – Higher order corrections

• Uncertainty quantification
  – Theoretical error from interaction
  – Errors from optimization and extrapolations
  – Theoretical error from manybody calculations

• (Grand) challenge problems
  – Neutrinoless double beta-decay
  – Limits of stability
  – Open-shell nuclei
Questions?

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